

COMPLETE STRUCTURE OF THE ANTI ROTAMER OF 1,1,2,2-TETRAFLUOROETHANE FROM INFRARED SPECTROSCOPY

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High-resolution (0.0018 cm^{-1}) infrared spectra have been recorded in the CF stretching region for 1,1,2,2-tetrafluoroethane and its d_2 and $^{13}\text{C}_2$ isotopomers. These bands are sufficiently intense to give useful gas-phase spectra at -100°C in a 3-m cell. For each spectrum the rotational structure of the A/C-type and B-type bands due to the anti rotamer, which is a highly asymmetric rotor with $\kappa = -0.295$, have been analyzed. Rotational constants for a Watson-type Hamiltonian have been fitted for the common ground state of each isotopomer and the separate upper states. A complete structure for the nonpolar anti rotamer has been derived and compared with the structure of the polar gauche rotamer obtained from microwave spectroscopy. The geometric parameters for the two rotamers are compared with recent calculations, and trends in these parameters are discussed.